

Empirical relations for the field dependence of electron mobility in InSb

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Abstract : The electron mobility has been obtained in InSb by the Monte Carlo simulation technique for different applied electric fields. The mobility values have then been expressed empirically by simple power law relationship. It is observed that the mobility values calculated by using these simple power law relations yield values that show agreement within 5% with those obtained from the detailed Monte Carlo simulation technique. It is concluded that these empirical relations can be used effectively for a quick estimation of mobility, as a check on experiments and also as sufficiently accurate formulae for simulation and modelling purposes.

Keywords : Indium antimonide, Monte Carlo simulation, electron mobility

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Indium Antimonide(InSb) is a widely used material for solid state electronic devices. Electron mobility in this material has been obtained using the displaced Maxwellian distribution function under different physical conditions [1-4]. The analytical methods for obtaining the conduction properties in semiconductors is beset with many complications. Various approximations not all of which can be justified, have to be used to bypass these difficulties under high field conditions. The Monte Carlo (MC) technique provides a better and more rigorous solution in such a situation. The MC simulation method has become a standard numerical technique for theoretical studies of the electron mobility as well as transport properties of hot carriers in semiconductors. With this in mind, we present in this note, a simple functional relationship between the electron mobility and the electric field in InSb at 77K for different impurity concentration. The mobility values have been calculated at different electric fields by the Monte Carlo (MC) simulation technique. The mobility values are then expressed by simple power law relationships, the coefficients of which are determined by a Least Mean Square Fit (LMSF) technique.

The Monte Carlo Simulation Technique for the calculation of electron transport parameters in a semiconductor has already been described in detail [5 - 7]. Here, the electron mobility has been calculated in InSb at 77K for electric fields up to 1 KV/cm by the Monte Carlo Simulation Technique.

In this technique, the carrier is presumed to start with an initial wave vector k_0 . Under the influence of the external electric field, it accelerates and continues its motion in what is called its free flight. The duration of the free flight is estimated by a pseudo-random number r_0 distributed uniformly between 0 and 1. The time at which the collision takes place is given by

$$t_c = -(\ln r_0)/\Gamma,$$

where Γ is the chosen Rees' parameter. Γ has been rendered constant over the energy range considered by including a self-scattering term such that the sum of all the real scattering rates plus the self-scattering rate remains constant over the entire energy range considered. It has been shown that the steady state value obtained by including the self-scattering term is indeed the value corresponding to the real scatterings. The wave vector of the carrier at the end of the free flight is k and this is computed by using the laws of classical mechanics. Once t_c is

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determined, one may obtain the trajectory of the electron from 0 to t_c by using the laws of Newtonian mechanics.

Having determined the instant at which the free flight has been terminated, one has to determine the type of collision that terminated the free flight. The scattering rates S_i corresponding to the various scattering mechanisms for the carrier with wave vector k are then computed by using the expressions detailed in Ref. [9]. Next, another random number r_1 is used to ascertain which one of the n scattering mechanisms including the self scattering processes has been operative. The j^{th} mechanism is chosen to terminate the free flight, if

$$\sum_{i=1}^j S_i / \sum_{i=1}^n S_i \leq r_1 < \left(\sum_{i=1}^{j+1} S_i / \sum_{i=1}^n S_i \right). \quad (1)$$

Having determined the kind of scattering, the energy and the wave vector of the electron after a real collision are determined from the conservation of the energy and the momentum. The energy of the electron after collision is given by $E + \Delta E$, where ΔE is the change in energy induced by the collision and E is the energy of the electron immediately before the collision. It is given by

$$E = \hbar^2 k^2 (t_c / 2m^*). \quad (2)$$

For acoustic, piezoelectric and ionized impurity scatterings, ΔE is taken equal to zero, while for polar optical phonon scattering, it is equal to $\pm \hbar \omega_1$.

The magnitude of the electron wave vector after the collision is then given by

$$k_i = [2m^* (E + \Delta E)]^{1/2} / \hbar. \quad (3)$$

This value of the wave vector is taken as the initial wave vector for the next free flight.

The orientation of the wave vector after collision is obtained by generating two more random numbers r_2 and r_3 , distributed uniformly between 0 and 1. We note that the probability that the polar angle θ and the azimuthal angle ϕ of the wave vector k_i with respect to any convenient direction, will be contained in the intervals $d\theta$ and $d\phi$ is proportional to $\sin \theta d\theta d\phi$. θ and ϕ can therefore, be chosen with the random numbers r_2 and r_3 as

$$\cos \theta = 1 - 2r_2, \quad \phi = 2\pi r_3. \quad (4)$$

The average velocity can be obtained from displacement and time by dividing the total displacement along the field direction by the total time.

$$V_z = (\hbar/m^*) \sum_i \left(k_{zi} t_{ci} + \left(\frac{eE}{\hbar} \right) \left(\frac{t_{ci}^2}{2} \right) \right) / \sum_i t_{ci}. \quad (5)$$

The average velocity can also be obtained from energy and momentum

$$V_d = \hbar^{-1} \sum (E_f - E_i) / \sum (k_{fz} - k_{iz}),$$

where E_i and E_f are respectively the energy after a collision and before the next collision. k_{iz} and k_{fz} are the corresponding components of the wave vector in the field direction. It is to be noted that the velocity values obtained by using the above two methods agree exactly with each other. Then the mobility values have been obtained for various electric fields. The results obtained from the calculations by MC technique are in close agreement with the available experimental data. The program for Monte Carlo simulation is written in C and the material parameters used are

$$m^*/m_0 = 0.0146, \quad \kappa_0 = 17.88, \quad \kappa_\alpha = 15.68, \quad \rho = 5.77 \text{ gm cm}^{-3}, \\ \theta_D = 292 \text{ K}, \quad K_m^2 = 0.027, \quad E_g = 0.24 \text{ eV}, \quad \Delta = 0.9, \quad E_1 = 30 \text{ eV}$$

The empirical relations between electron mobility μ and the applied electric field E has been taken to be of the form

$$\mu = a_0 + a_1 E + a_2 E^2 + a_3 E^3 \quad (6)$$

It has been found that by retaining terms upto the 3rd order the empirical relations give values accurate to within 5% of the values obtained from the detailed MC simulation technique. The values of the coefficients a_0 , a_1 , a_2 and a_3 as calculated from the Least-Mean-Square fit of mobility are given in Table 1.

Table 1. Values of coefficients for Least-Mean-Squares fit of mobility in InSb.

Ionized impurity concentration	a_0 cm ² /kV.sec	a_1 cm ³ / (kV) ² .sec	a_2 cm ⁴ / (kV) ³ .sec	a_3 cm ⁵ / (kV) ⁴ .sec
0	59.6886	- 164.102	193.974	- 83.666
10^{14}	53.3849	- 131.641	145.1815	- 59.704
5×10^{14}	39.0484	- 84.145	79.425	- 28.182

We have plotted in Figure 1 the values of the electron mobility in InSb, calculated by the MC simulation technique and by using the empirical relation (6), for different values of the applied electric field and impurity concentration. It is seen that the results obtained by MC simulation technique and empirical relation agree quite satisfactorily. A device modelling program requires the mobility values to be evaluated at a large number of applied electric field. In such a case, the empirical relationship given in relation (1) can be put to use effectively without any loss of accuracy while keeping the computer time insignificant compared to that necessary for a detailed MC simulation technique at all those fields.

It is concluded that the relation (1) between mobility and electric field obtained by the least mean square fit technique will be useful for quick estimation of mobility in non-parabolic semiconductors under high field conditions without having to take recourse to detailed Monte Carlo simulation technique in

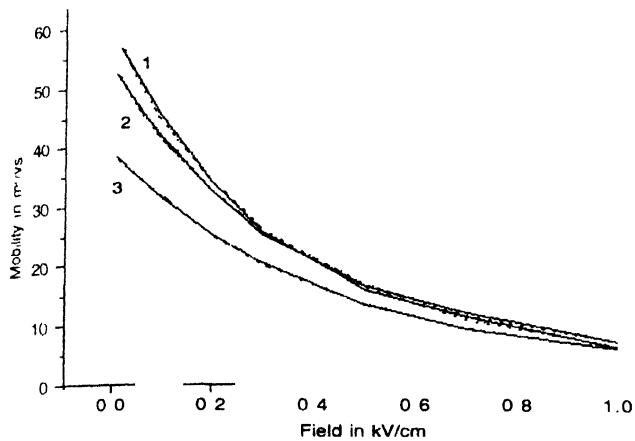


Figure 1. Variation of electron mobility with applied electric field at 77 K for InSb at different ionized impurity concentrations (1) $N_i = 0$, (2) $N_i = 1e14$, (3) $N_i = 5e14$. Solid line: MC Simulation, Dotted line: Estimation using eq. (1).

device simulation and for a quick comparison of experimental data with theoretical results.

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